

EMLG2022 POSTERS LIST

Abdullah Ahmad (University of Strathclyde, UK) <i>pyRISM – Python Implementation of the Reference Interaction Site Model</i>	17
Aymeric Allemand (Institute of Light and Matter (ILM), France) <i>Ionic transport in soft subnanometric films</i>	4
László Almásy (Centre for Energy Research, Hungary) <i>Structure of Aqueous Solutions of Heterocyclic Amines</i>	37
Edgar Alvarez Galera (Universitat Politècnica de Catalunya, Spain) <i>Nucleation of helium in molten lithium</i>	42
Roi Bar-On (Technion, Israel) <i>Theory for Heterogeneous Water/Oil Separation</i>	38
Roger Bellido Peralta (Universitat de Barcelona, Spain) <i>Water-methanol mixture segregation and separation under confinement</i>	5
Samuel Blazquez (Complutense University of Madrid, Spain) <i>The Madrid-2019 force field for electrolytes in water: An extension to the ions F⁻, Br⁻, I⁻, Rb⁺ and Cs⁺</i>	19
Dezso Boda (University of Pannonia, Hungary) <i>Rules of thumb for creating useful reduced models: the case study of nanopores</i>	1
Carles Calero (Universitat de Barcelona, Spain) <i>Dynamics of water under confinement by soft and hard boundaries: a comparative analysis using all-atom MD simulations.</i>	6
Manel Canales (Universitat Politècnica de Catalunya, Spain) <i>Hydrogen bonding in aqueous solutions of sulfuric and methanesulfonic acids: a computer simulation study</i>	20
Frédéric Caupin (University Lyon 1, France) <i>Fluid phase equilibrium in confinement: effects of compressibility and wetting</i>	7
Luis Enrique Coronas (University of Barcelona, Spain) <i>A quantitative water model for large-scale simulations at life-relevant conditions</i>	21
Joanna Feder-Kubis (Wroclaw University of Science and Technology, Poland) <i>Task-specific ionic liquids as smart additives for nanoparticles</i>	12
Nadia Figueiredo (University of Porto, Portugal) <i>Anion-based magnetic ionic liquids: from non-polarizable to polarizable force fields</i>	13
Jordi Fraxedas (ICN2, Spain) <i>Radial and unidirectional water pumping using zeta-potential modulated Nafion nanostructures</i>	43
Francisco Gámez (Universidad Complutense de Madrid, Spain) <i>Experimental and simulation results (using the extended Madrid-2019 force field) for the maximum in density of 1m salt solutions containing the cations Rb⁺ and Cs⁺: and the anions F⁻, Br⁻ and I⁻.</i>	22
Joanna Grabowska (Universidad Complutense de Madrid, Spain) <i>Solubility of methane in water and its connection to the hydrate nucleation</i>	23

Elvira Guardia (Universitat Politècnica de Catalunya, Spain) <i>Fingerprints of the crossing of the Frenkel and Melting Lines in high-pressure supercritical water</i>	47
Myroslav Holovko (Institute for Condensed Matter Physics, Ukraine) <i>One hundred years for Enskog theory: application to fluids in porous media</i>	8
Shinya Hosokawa (Kumamoto University, Inst. Industrial Nanomaterials, Japan) <i>Improved Data Analysis on Atomic Dynamics in Liquid CCl₄</i>	44
Zheyao Hu (Polytechnic University of Catalonia-Barcelona Tech, Spain) <i>The Crucial role of Mg₂₊ in conformational change of KRas</i>	2
Lasse Hunger (University Rostock, Germany) <i>The fragmentation of intermolecular interactions in a carboxyl-functionalized ionic liquid and its molecular mimic – Quantification of hydrogen bond strength</i>	14
Akos Juhasz (University of Lille, France) <i>Characterizing electrospun 3D matrices for biomedical purposes</i>	34
Ivo Jukic (University of Split, Croatia (Hrvatska)) <i>Universality of two gigahertz-ranged cluster lifetimes in hydrogen bonding liquids and mixtures</i>	39
Arnau Jurado Romero (Universitat Politècnica de Catalunya, Spain) <i>Vibrational cooling dynamics of nitromethane</i>	24
David Kotwica (University of Rostock, Germany) <i>Spectroelectrochemical and IR-photocatalytic investigations of manganese based CO₂-reduction-catalysts</i>	35
Yuting Li (Khalifa University, United Arab Emirates) <i>Computational screening of Transition metals doped on CdS photocatalyst for green hydrogen generation</i>	25
Narayan Chandra Maity (S N Bose National Centre for Basic Sciences, India) <i>Spatio-temporal heterogeneity in octanol rich region: Revealing via time resolved fluorescence measurements</i>	45
Gionni Marchetti (Universitat de Barcelona, Spain) <i>Can Machine Learning help us to systematically analyze the UV Resonance Raman Spectra of Glycoproteins absorbing on Nanoparticles?</i>	36
Jordi Marti (UPC, Spain) <i>Oncogenic K-Ras Proteins: Mechanisms of Activation by Guanine Exchange Factors</i>	40
Fatima Matroodi (Elettra Sincrotrone, Italy) <i>Hydrogen bonding and local structure of imidazolium-based ionic liquids in water</i>	15
Jayanta Mondal (S N Bose National Centre for Basic Sciences, India) <i>Temperature dependent dielectric relaxation measurement of an amino acid derivative based deep eutectic solvent: origin of timescales via experiment and molecular dynamics simulation</i>	41
Ana Maria Montero (University of Extremadura, Spain) <i>Equation of state of hard-disk fluids under single-file confinement</i>	9
Jule Kristin Philipp (University of Rostock, Germany) <i>Cluster Formation in Mixtures of [Li][NTf₂] and Triglyme</i>	26

Milan Predota (University of South Bohemia, Czech Republic) <i>Vibrational SFG spectrum prediction from classical molecular dynamics simulations</i>	27
Farid Rizk (Institut Lumière Matière, France) <i>Microscopic origins of the viscosity of a Lennard-Jones liquid</i>	28
Zsófia Judit Sarkadi (University of Pannonia, Hungary) <i>Scaling for selectivity in uniformly charged selective nanopores</i>	10
Ari Paavo Seitsonen (Ecole normale supérieure - CNRS, France) <i>Quercetin in water, studied with molecular simulations</i>	3
Abderrahmane Semmeq (Université de Lorraine-CNRS, France) <i>Tuning the Optical Properties of a Chromophore in a Nanoconfined Environment</i>	29
Gemma Sesé (Universitat Politècnica de Catalunya, Spain) <i>The 2PT approach for a molecular dipolar liquid</i>	30
Mohd Rafie bin Shaharudin (The University of Manchester, UK) <i>The role of surface ionisation in the hydration-induced swelling of graphene oxide membrane</i>	31
Shokirbek Shermukhamedov (Institute of Ion Physics and Applied Physics, University of Innsbruck, Austria) <i>Heterogeneous Electron Transfer Reactions inside Carbon Nanotubes: Molecular Dynamics Simulations</i>	32
Jiri Skvara (Jan Evangelista Purkyně University in Ústí nad Labem, Czech Republic) <i>Thermodynamics and structure of TIP4P/Ice supercooled water</i>	46
Michika Takeda (Kyushu University, Japan) <i>Calculation of effective interaction between like-charged particles; The HNC-OZ theory and Monte Carlo simulation</i>	16
Mónika Valiskó (University of Pannonia, Hungary) <i>The Mean Countershell Approximation (MCSA) theory for the excess chemical potential of electrolytes: comparison to Monte Carlo simulations</i>	18
Maria von Einem (University of Bremen, Germany) <i>Is TiO₂ cleaning our wastewater in the future?</i>	33
Zixuan Wei (The University of Manchester, UK) <i>Wettability of graphite under 2D confinement</i>	11

Posters Schedule:

Posters should be displayed on Tuesday September 13, 2022 (before the morning coffee break) and should be removed Friday September 16, 2022 (after the morning coffee break).